CLASE 22 - Viernes 18/06/2021

La clase pasada vimos:

Elemento de matriz del dipolo eléctrico

Ecuación de movimiento de la polarización interbanda

Polarización interbanda de partícula libre

En esta clase veremos:

Ecuación de Wannier

Excitones de Wannier

REPASO

Ecuación de movimiento de la **polarización interbanda**

Modelo de dos bandas

$$\hbar\left[i\frac{d}{dt}-(\epsilon_{c,k}-\epsilon_{v,k})\right]P_{vc,\mathbf{k}}(t)=\left[n_{c,\mathbf{k}}(t)-n_{v,\mathbf{k}}(t)\right]d_{cv}\mathcal{E}(t)$$
$$+\sum_{\mathbf{k}',\mathbf{q}\neq 0}V_q\Big(\langle a^\dagger_{c,\mathbf{k}'+\mathbf{q}}a^\dagger_{v,\mathbf{k}-\mathbf{q}}a_{c,\mathbf{k}'}a_{c,\mathbf{k}}\rangle+\langle a^\dagger_{v,\mathbf{k}'+\mathbf{q}}a^\dagger_{v,\mathbf{k}-\mathbf{q}}a_{v,\mathbf{k}'}a_{c,\mathbf{k}}\rangle$$
$$+\langle a^\dagger_{v,\mathbf{k}}a^\dagger_{c,\mathbf{k}'-\mathbf{q}}a_{c,\mathbf{k}'}a_{c,\mathbf{k}-\mathbf{q}}\rangle+\langle a^\dagger_{v,\mathbf{k}}a^\dagger_{v,\mathbf{k}'-\mathbf{q}}a_{v,\mathbf{k}'}a_{c,\mathbf{k}-\mathbf{q}}\rangle\Big)\quad,$$

Incógnitas:

$$\begin{cases} P_{vc,\mathbf{k}}(t)=\langle a^\dagger_{v,\mathbf{k}}a_{c,\mathbf{k}}(t)\rangle \\ n_{\lambda,\mathbf{k}}=\langle a^\dagger_{\lambda,\mathbf{k}}a_{\lambda,\mathbf{k}}\rangle \end{cases}$$

Bandas de energía del sólido:

$$\begin{cases} E_{c,k}=\hbar\epsilon_{c,k}=E_g+\hbar^2k^2/2m_c \\ E_{v,k}=\hbar\epsilon_{v,k}=\hbar^2k^2/2m_v \end{cases}$$

Polarización: $P(t)=\sum_{\mathbf{k}}P_{cv,\mathbf{k}}(t)d_{vc}+\text{c.c.}$

REPASO

Ecuación de movimiento de la **polarización interbanda** en la Random-Phase Approximation (RPA)

$$\hbar\left[i\frac{d}{dt}-(e_{c,k}-e_{v,k})\right]P_{vc,\mathbf{k}}(t)$$
$$=\left[n_{c,\mathbf{k}}(t)-n_{v,\mathbf{k}}(t)\right]\left[d_{cv}\mathcal{E}(t)+\sum_{\mathbf{q}\neq\mathbf{k}}V_{|\mathbf{k}-\mathbf{q}|}P_{vc,\mathbf{q}}\right]. \qquad (10.21)$$

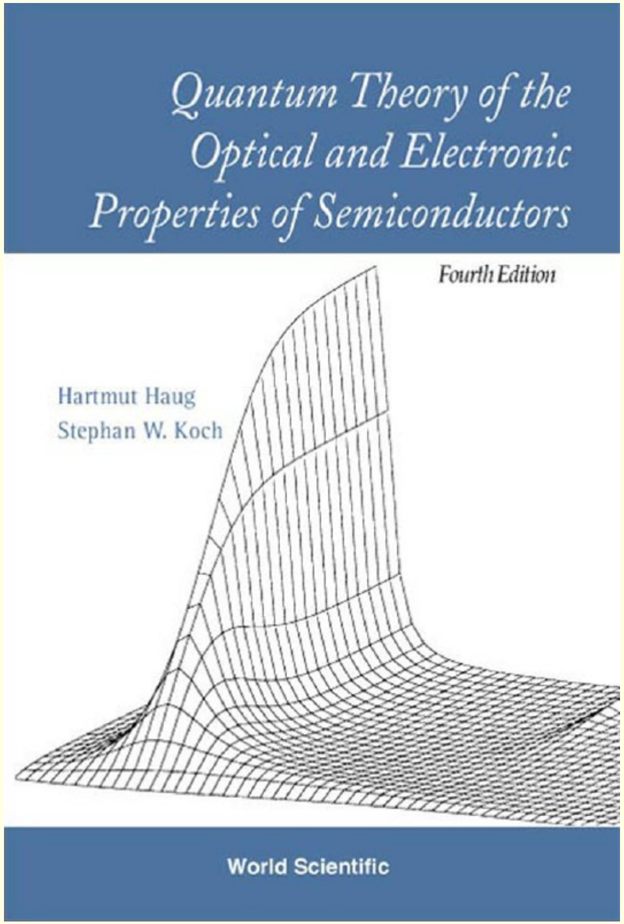
dynamics of interband polarization (pair) function

$$\boxed{e_{\lambda,\mathbf{k}}=\epsilon_{\lambda,\mathbf{k}}+\Sigma_{exc,\lambda}(\mathbf{k})}$$

Energías de partícula única renormalizadas

$$\hbar\Sigma_{exc,\lambda}(k)=-\sum_{\mathbf{q}\neq\mathbf{k}}V_{|\mathbf{k}-\mathbf{q}|}n_{\lambda,\mathbf{q}}$$

Auto-energías en aproximación de Hartree-Fock



10. Excitons 163

10.1 The Interband Polarization 164
10.2 Wannier Equation 169
10.3 Excitons 173
10.3.1 Three- and Two-Dimensional Cases 174
10.3.2 Quasi-One-Dimensional Case 179

12. Semiconductor Bloch Equations 211

Ecuación de Wannier

Ecuación de Wannier

$$\hbar\left[i\frac{d}{dt}-(e_{c,k}-e_{v,k})\right]P_{vc,\mathbf{k}}(t)=(f_{c,\mathbf{k}}-f_{v,\mathbf{k}})\left[d_{cv}\mathcal{E}(t)+\sum_{\mathbf{q}\neq\mathbf{k}}V_{|\mathbf{k}-\mathbf{q}|}P_{vc,\mathbf{q}}\right]$$

La respuesta lineal corresponde a: $f_{c,k}\equiv 0 \quad \text{and} \quad f_{v,k}\equiv 1$

(semiconductor no excitado)

Tomando transformada de Fourier (tiempo):

$$\left[\hbar(\omega+i\delta)-E_g-\frac{\hbar^2k^2}{2m_r}\right]P_{vc,\mathbf{k}}(\omega)=-\left[d_{cv}\mathcal{E}(\omega)+\sum_{\mathbf{q}\neq\mathbf{k}}V_{|\mathbf{k}-\mathbf{q}|}P_{vc,\mathbf{q}}(\omega)\right]$$

$$\frac{1}{m_r}=\frac{1}{m_c}-\frac{1}{m_v}$$

Ecuación de Wannier

$$\left[\hbar(\omega+i\delta)-E_g-\frac{\hbar^2k^2}{2m_r}\right]P_{vc,\mathbf{k}}(\omega)=-\left[d_{cv}\mathcal{E}(\omega)+\sum_{\mathbf{q}\neq\mathbf{k}}V_{|\mathbf{k}-\mathbf{q}|}P_{vc,\mathbf{q}}(\omega)\right]\ , \quad (10.31)$$

Tomando transformada de Fourier (espacio):

$$\frac{L^3}{(2\pi)^3}\int d^3k\ldots$$

$$f(\mathbf{r}) = \frac{L^3}{(2\pi)^3}\int d^3q f_{\mathbf{q}} e^{-i\mathbf{q}\cdot\mathbf{r}}$$

$$f_{\mathbf{q}} = \frac{1}{L^3}\int d^3r f(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}}$$

$$\left[\hbar(\omega+i\delta)-E_g+\frac{\hbar^2\nabla_{\mathbf{r}}^2}{2m_r}+V(r)\right]P_{vc}(\mathbf{r},\omega)=-d_{cv}\mathcal{E}(\omega)\,\delta(\mathbf{r})L^3 \quad (10.34)$$

Ecuación de Wannier

$$\left[\hbar(\omega + i\delta) - E_g + \frac{\hbar^2 \nabla_{\mathbf{r}}^2}{2m_r} + V(r)\right] P_{vc}(\mathbf{r}, \omega) = -d_{cv}\mathcal{E}(\omega)\,\delta(\mathbf{r})L^3 \qquad (10.34)$$

Consideremos la ecuación homogénea:

$$-\left[\frac{\hbar^2 \nabla_{\mathbf{r}}^2}{2m_r} + V(r)\right] \psi_\nu(\mathbf{r}) = E_\nu \psi_\nu(\mathbf{r})$$

ECUACIÓN DE WANNIER

Donde identificamos:

$$\begin{cases} P_{vc}(\mathbf{r}, \omega) \longrightarrow \psi_\nu(\mathbf{r}) \\ \hbar(\omega + i\delta) - E_g \longrightarrow E_\nu \end{cases}$$

Ecuación de Wannier

$$-\left[\frac{\hbar^2\nabla_{\mathbf{r}}^2}{2m_r}+V(r)\right]\psi_\nu(\mathbf{r})=E_\nu\psi_\nu(\mathbf{r})$$

Masa reducida: protón → hueco (masa efectiva)

$$\frac{1}{m_r}=\frac{1}{m_c}-\frac{1}{m_v}$$

$$m_v<0$$

Sistema hidrogenoide

$$V(r)=\frac{e^2}{\epsilon_0 r}$$

Background dielectric constant

Solución de la ecuación de Wannier

Solución de la ecuación de Wannier

$$-\left[\frac{\hbar^2 \nabla_{\mathbf{r}}^2}{2m_r} + V(r)\right]\psi_\nu(\mathbf{r}) = E_\nu \psi_\nu(\mathbf{r})$$

Rescaleo la distancia: $\rho = r\alpha$

$$\left(-\nabla_\rho^2 - \frac{\lambda}{\rho}\right)\psi(\rho) = \frac{2m_r E_\nu}{\hbar^2\alpha^2}\psi(\rho)$$

Donde: $\lambda = \dfrac{e^2 2m_r}{\epsilon_0 \hbar^2 \alpha} = \dfrac{2}{\alpha a_0}$

Solución de la ecuación de Wannier

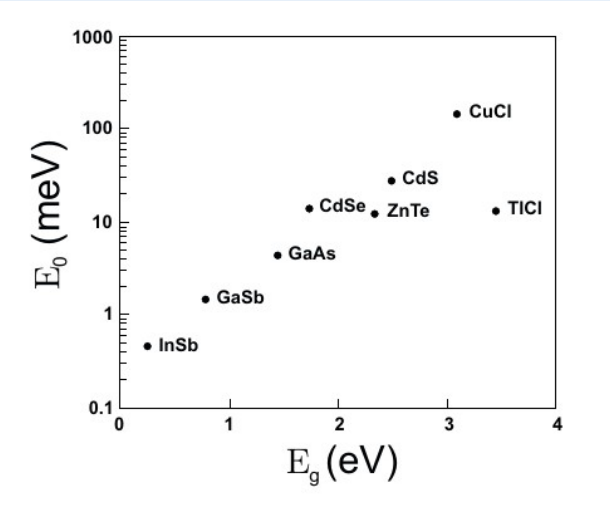
Radio de Bohr renormalizado:

$$a_0 = \frac{\hbar^2 \epsilon_0}{e^2 m_r}$$

Rydberg renormalizado:

$$E_0 = \frac{\hbar^2}{2 m_r a_0^2} = \frac{e^2}{2\epsilon_0 a_0} = \frac{e^4 m_r}{2\epsilon_0^2 \hbar^2}$$

Binding energy experimental:



Solución de la ecuación de Wannier

Se puede plantear el problema en 3D, 2D y 1D.

El Laplaciano depende de la dimensionalidad:

$$\nabla_\rho^2 = \frac{1}{\rho^2}\frac{\partial}{\partial\rho}\rho^2\frac{\partial}{\partial\rho} - \frac{\mathcal{L}^2}{\rho^2} \qquad \text{in } 3D$$

$$\nabla_\rho^2 = \frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} - \frac{\mathcal{L}_z^2}{\rho^2} \qquad \text{in } 2D$$

$$\nabla_\rho^2 = \frac{\partial^2}{\partial\zeta^2} \qquad \text{in } q1D$$

$$\begin{aligned} \psi(\rho) &= f_l(\rho) Y_{l,m}(\theta,\phi) && \text{in } 3D \\ &= f_m(\rho)\frac{1}{\sqrt{2\pi}}e^{im\phi} && \text{in } 2D \end{aligned}$$

Excitones

Excitones

Ecuación del sistema hidrogenoide adimensionalizado :

$$\left(\frac{1}{\rho^2}\frac{\partial}{\partial\rho}\rho^2\frac{\partial}{\partial\rho}+\frac{\lambda}{\rho}-\frac{1}{4}-\frac{l(l+1)}{\rho^2}\right)f_l(\rho)=0 \quad \text{in} \quad 3D$$

$$\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}+\frac{\lambda}{\rho}-\frac{1}{4}-\frac{m^2}{\rho^2}\right)f_m(\rho)=0 \quad \text{in} \quad 2D$$

Las soluciones **ligadas** son los **excitones de Wannier**.

$$\boldsymbol{E_n = -E_0\frac{1}{n^2}} \quad \text{with } \boldsymbol{n = 1, 2, \ldots}$$

$3D$ exciton bound-state energies

$$\boldsymbol{E_n = -E_0\frac{1}{(n+1/2)^2}} \quad \text{with } \boldsymbol{n = 0, 1, \ldots ,}$$

$2D$ exciton bound-state energies

ν_{max}	n	l	$f_{n,l}(\rho) = C\rho^l e^{-\frac{\rho}{2}} \sum_\nu \beta_\nu \rho^\nu$	E_n
0	1	0	$f_{1,0}(r) = \frac{1}{a_0^{3/2}} 2\, e^{-r/a_0}$	$E_1 = -E_0$
1	2	0	$f_{2,0}(r) = \frac{1}{(2a_0)^{3/2}}(2 - \frac{r}{a_0})e^{-r/2a_0}$	$E_2 = -\frac{E_0}{4}$
0	2	1	$f_{2,1}(r) = \frac{1}{(2a_0)^{3/2}} \frac{r}{\sqrt{3}a_0} e^{-r/2a_0}$	$E_2 = -\frac{E_0}{4}$.

(10.67)

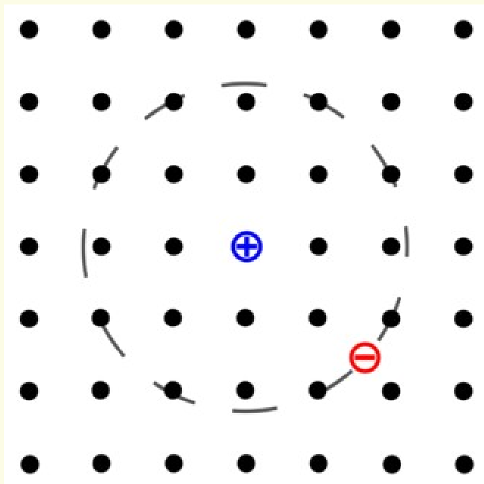
$3D$ radial exciton wave functions

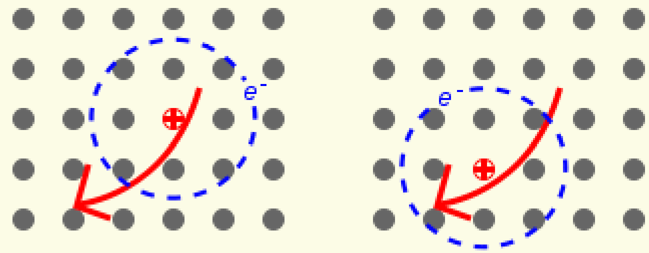
ν_{max}	n	m	$f_{n,m}(\rho) = C\rho^{\|m\|}e^{-\frac{\rho}{2}}\sum_\nu \beta_\nu \rho^\nu$	E_n
0	0	0	$f_{0,0}(r) = \frac{1}{a_0}4e^{-2r/a_0}$	$E_{n=0} = -4E_0$
1	1	0	$f_{1,0}(r) = \frac{4}{a_0 3\sqrt{3}}\left(1 - \frac{4r}{3a_0}\right)e^{-\frac{2r}{3a_0}}$	$E_1 = -\frac{4E_0}{9}$
0	1	± 1	$f_{1,\pm 1}(r) = \frac{16}{a_0 9\sqrt{6}}\frac{r}{a_0}e^{-2r/3a_0}$	$E_1 = -\frac{4E_0}{9}$.

(10.68)

2D radial exciton wave functions

Excitones de Frenkel





Excitones de Frenkel
Materiales con constante dieléctrica chica,
Energía grande, radio chico, fijos.

Excitones de Wannier
Radio grande, energía baja, móviles.

Resumen de la clase 21

Ecuación de Wannier

Excitones de Wannier